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Title: Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

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Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

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Stress and Strain

- Body B (reference configuration/frame), region $\mathcal{E}$.
  Material points $p \in \mathrm{B}$.
- Deformation: a mapping f such that $x = f(p)$.
- Displacement: $u(p) = f(p) - p$.
- Deformation gradient: $F(p) = \nabla f(p)$.
- Strain: there are many.
  Eg. Infinitesimal strain, $\varepsilon = \frac{1}{2}(\nabla u + \nabla u^T)$.

  - Elastic strain, inelastic strain.
  - Total strain = elastic strain + inelastic strain, for certain strains.
- Stress:
  - Forces that tend to return the body to equilibrium when deformation occurs, i.e. no deformation means no stress.
  - The sum of the forces exerted on the body by its surrounding, i.e. surface integral of the external forces.

Stress and Strain

- Constitutive laws: the relationship between stress and strain.

  - Hyperelasticity: ∃ potential function of which derivative with respect to elastic strain is stress as a result of Clausius-Duhem (the second law of thermodynamics).
  - Hypoelasticity: no such potential.
  - Flow stress models (also called strength models): Stress that is required to deform the material plastically.

    Relates stress and plastic strain (and possibly other things like plastic strain rates and temperature).
  - Equation of State: relates the equilibrium thermodynamic quantities like volume, pressure, internal energy, entropy, temperature, etc.
  - Elastic strain ~ volumetric

    Plastic strain ~ non-volumetric or deviatoric.

Flow Stress Models

- Flow stress as a function of strain, strain rate, and temperature.
- Johnson-Cook

$$\sigma_y(\epsilon_p, \dot{\epsilon}_p, T) = [A + B(\epsilon_p)^n] \left[1 + C \ln(\dot{\epsilon}_p^*)\right] [1 - (T^*)^m]$$

- Steinberg-Cochran-Guinan-Lund

$$\sigma_y(\epsilon_p, \dot{\epsilon}_p, T) = [\sigma_a f(\epsilon_p) + \sigma_t(\dot{\epsilon}_p, T)] \frac{\mu(p, T)}{\mu_0}; \quad \sigma_a f \leq \sigma_{\max} \text{ and } \sigma_t \leq \sigma_p$$

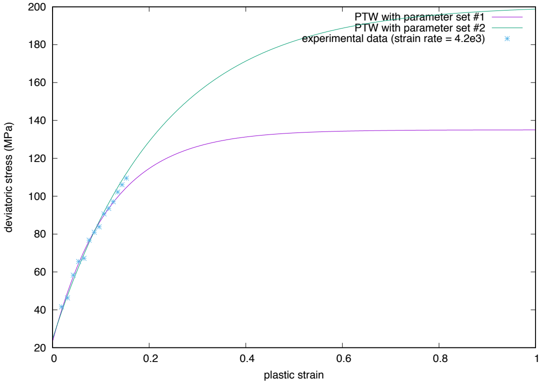
$$f(\epsilon_p) = [1 + \beta(\epsilon_p + \epsilon_{pi})]^n$$

- Mechanical Threshold Stress

$$\sigma_y(\epsilon_p, \dot{\epsilon}_p, T) = \sigma_a + (S_i \sigma_i + S_e \sigma_e) \frac{\mu(p, T)}{\mu_0}$$

Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

- Specifies the flow stress as a function of strain, strain rate, and temperature.
- Applicable to a wide range of strain rate (from 1e-3/s to 1e+12/s).
  In the low strain-rate regime, based on thermal-activation of dislocations;
  at high strain-rate, uses D. Wallace's theory of overdriven shocks in metals.
- Isotropic model without accounting for the loading history or microstructure.
- Modified Voce hardening law.
- Data needed for parameter fitting: split-Hopkinson pressure bar experiments (- 1e+4/s), quasi-static experiments (1e-3/s – 1/s).
- Insufficient data leads to the under-constrained parameters (total 11, usually 8 are fitted).
- J. Plohr et al. "The PTW Parameterization of Cerium," WRL 45, Mar 2018.



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Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

- Normalized (equivalent deviatoric) Stress as a function of normalized (equivalent deviatoric) strain and normalized temperature.
- $\hat{\sigma} = \hat{\sigma}(\hat{T}, \varepsilon;\ \dot{\varepsilon}/\dot{\xi}),$

  $\hat{\sigma} = \frac{\sigma}{2G}, G$: shear modulus; $\hat{T}$=T/T_m, T_m: melt temperature.
  - Stress – normalized by 2 x shear modulus (function of density and temperature).
  - Strain rate – normalized by ~ the debye frequency (equivalently the atomic vibration time).
  - Temperature – normalized by melt temperature (function of density).
- Need models (or tables) for shear modulus and melt temperature

$$G(\rho, T) = G_0(\rho)(1 - \alpha\, T/T_m)$$

$G_0(\rho)$: cold shear, i.e. shear modulus at zero temperature

- Need Equation of State
  - For thermodynamic consistency, $\dot{T} = -\Gamma T \frac{\dot{v}}{v} + \frac{v\sigma^{ij}\, \dot{\varepsilon}^{p}{}_{ij}}{C_v}$.

Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

- Normalized (equivalent deviatoric) Stress as a function of normalized (equivalent deviatoric) Strain and normalized Temperature.

$$\bar{\tau} = \bar{\tau}_s + \frac{1}{p}(s_0 - \bar{\tau}_y) \ln \left\{ 1 - \left[1 - \exp\left(-p \frac{\bar{\tau}_s - \bar{\tau}_y}{s_0 - \bar{\tau}_y} \right) \right] \exp\left[- \frac{p \theta \varepsilon^p}{(s_0 - \bar{\tau}_y)\left[\exp\left(p \frac{\bar{\tau}_s - \bar{\tau}_y}{s_0 - \bar{\tau}_y} \right) - 1 \right]} \right] \right\}$$

where $\bar{\tau}_s = \max\left\{ \bar{\tau}_s^L, \bar{\tau}_s^H \right\}$, $\bar{\tau}_y = \max\left\{ \bar{\tau}_y^L, \min\left\{ \bar{\tau}_y^M, \bar{\tau}_y^H \right\} \right\}$,

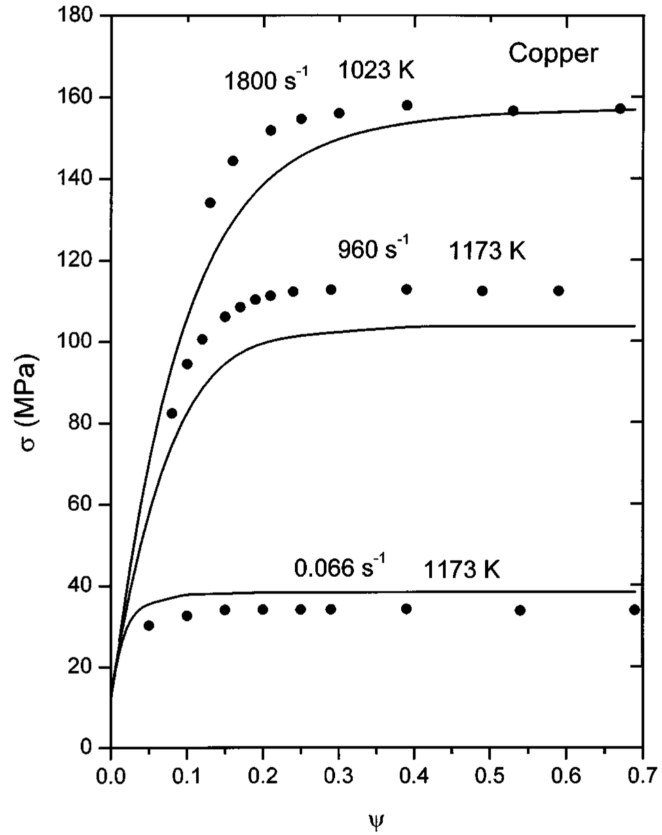
with $\bar{\tau}_s^L = s_0 - (s_0 - s_\infty)\,\mathrm{erf}\left[\kappa \bar{T} \ln\left(\frac{\gamma \dot{\xi}}{\dot{\varepsilon}^p} \right) \right]$, $\bar{\tau}_s^H = s_0 \left(\frac{\dot{\varepsilon}^p}{\gamma \dot{\xi}} \right)^{\beta}$,

$$\bar{\tau}_y^L = y_0 - (y_0 - y_\infty)\,\mathrm{erf}\left[\kappa \bar{T} \ln\left(\frac{\gamma \dot{\xi}}{\dot{\varepsilon}^p} \right) \right], \quad \bar{\tau}_y = \max\left\{ \bar{\tau}_y^L, \min\left\{ \bar{\tau}_y^M, \bar{\tau}_y^H \right\} \right\},$$

and $\bar{\tau}_y^M = y_1 \left(\frac{\dot{\varepsilon}^p}{\gamma \dot{\xi}} \right)^{y_2}$.

Preston-Tonks-Wallace (PTW) Visco-Plasticity Model

- For higher strain rate, the flow stress is higher.
- For lower temperature, the flow stress is higher.



Thermoelasticity Model

- L. Burakovsky, J. N. Plohr, S. K. Sjue, and D. J. Luscher, “Thermoelasticity Model for Cerium,” LA-UR-26990, 2017.
- Unified analytic melt-shear model to describe both the cold shear modulus and melting temperature as functions of density.
- Based on the experimental, low-pressure behavior and high-pressure one-component plasma (OCP) theory.

$$\gamma_G(\rho) = \frac{1}{2} + \frac{\gamma_1}{\rho^{1/3}} + \frac{\gamma_2}{\rho^{q_2}},$$

$$\gamma_{T_m}(\rho) = \frac{1}{2} + \frac{\gamma_1}{\rho^{1/3}} + \frac{\gamma_3}{\rho^{q_3}}.$$

$$\frac{d \ln G(\rho)}{d \ln \rho} = 2\gamma_G(\rho) + \frac{1}{3},$$

$$\frac{d \ln T_m(\rho)}{d \ln \rho} = 2\gamma_{T_m}(\rho) + \frac{1}{3}.$$

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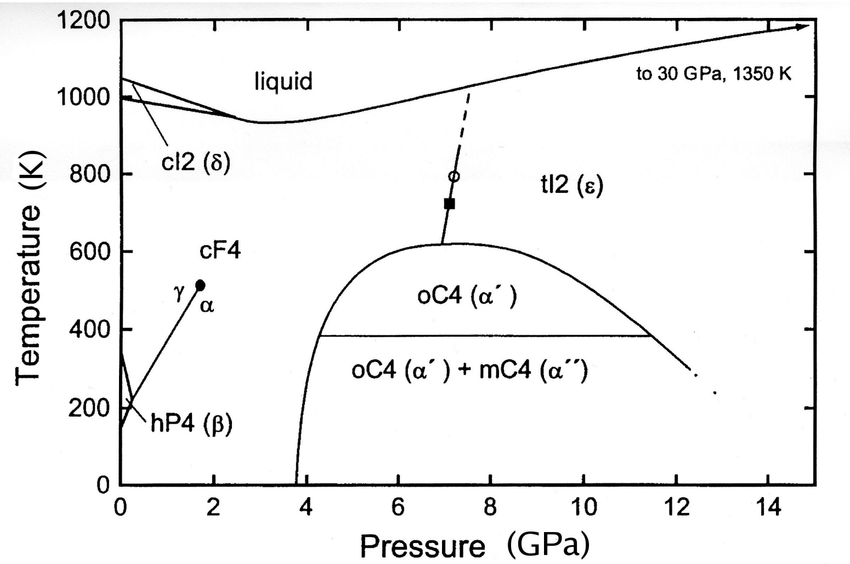
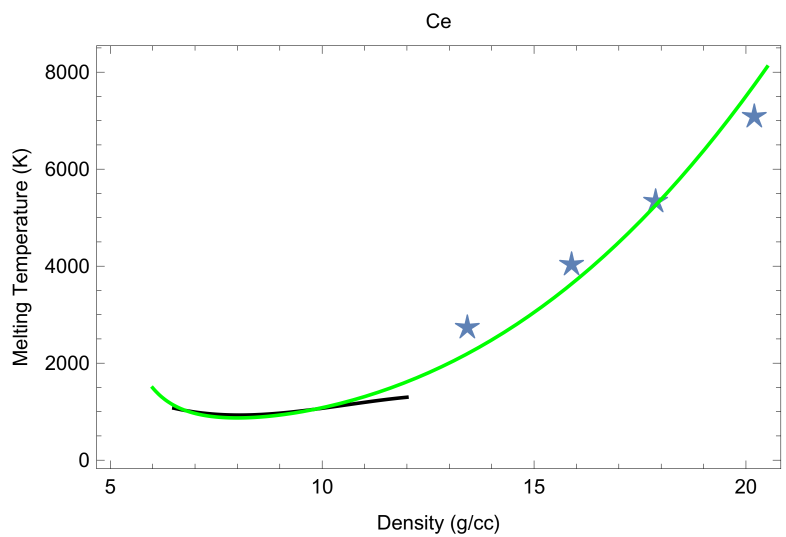
Multi-Phase Equation of State for Cerium

- Cerium (atomic number: 58) has 7 allotropes.
- Critical point at around 2 GPa and 500 K.
- Phase transformation between γ and α :
  - Localization/delocalization of 4f electron.
  - Big volume collapse: density $(\gamma) = 6.77\ \mathrm{g}/cm^3$, density $(\alpha) = 8.16\ \mathrm{g}/cm^3$.
  - Anomalous behavior of the bulk modulus -> wave profile.



Thermoelasticity Model

- $G(\rho) = G(\rho_0)\left(\frac{\rho}{\rho_0}\right)^{\frac{4}{3}} \exp\left\{-6\gamma_1\left(\rho^{-\frac{1}{3}} - \rho_0{}^{-\frac{1}{3}}\right) - \frac{2\gamma_2'}{q_2}\left(\rho^{-q_2} - \rho_0{}^{-q_2}\right)\right\},$
- $T_m(\rho) = T_m(\rho_m)\left(\frac{\rho}{\rho_m}\right)^{\frac{1}{3}} exp\left\{-6\gamma_1\left(\rho^{-\frac{1}{3}} - \rho_m{}^{-\frac{1}{3}}\right) - 3\gamma_2\left(\rho^{-\frac{2}{3}} - \rho_m{}^{-\frac{2}{3}}\right) - 2\gamma_3\left(\rho^{-1} - \rho_m{}^{-1}\right) - \frac{3}{2}\gamma_4\left(\rho^{-\frac{4}{3}} - \rho_m{}^{-\frac{4}{3}}\right)\right\}.$
- Parameters are fitted with the experimental data and quantum molecular dynamics (QMD) results.



Experimental Data for Cerium

- Split-Hopkinson pressure bar test done at Russian Federal Nuclear Center for the annealed cerium samples prepared at LANL.
- 7 distinct temperature/strain rate settings.

	Strain rate (/sec)	Temperature (K)	Number of tests
1	1000	293	3
2	3500	293	2
3	1000	333	2
4	3500	333	2
5	3500	373	2
6	1800	293	1
7	2500	373	1

Parameter Fitting

- J. Plohr et al. “The PTW Parameterization of Cerium,” WRL 45, March 2018.
- Higher strain data is needed for determining the asymptotic behavior.